Appl. No. 09/506,741; Group Art Unit: 1631
Dkt. No. 1503.0730000;
Inventor(s): Lobanov et al.; Tel: 202/371-2600
Title: System, Method and Computer Program Product for Past and Efficient Searching of Large Chemical Libraries

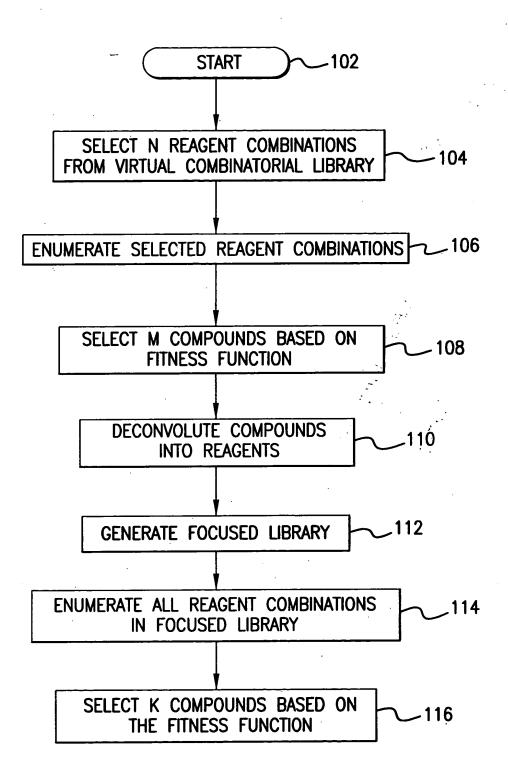
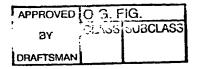


FIG.1



Appl. No. 09/506,741; Group Art Unit: 1631 Dkt. No. 1503.0730000; Inventor(s): Lobanov et al.; Tel: 202/371-2600 Title: System, Method and Computer Program Product for Fast and Efficient Searching of Large Chemical Libraries

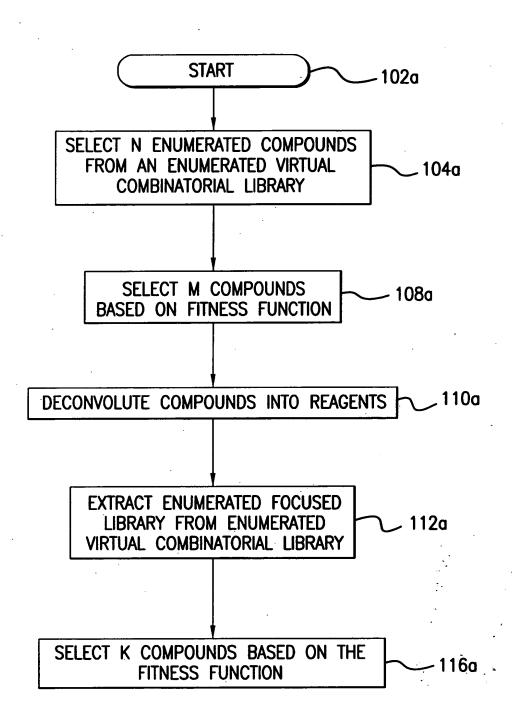


FIG.1A

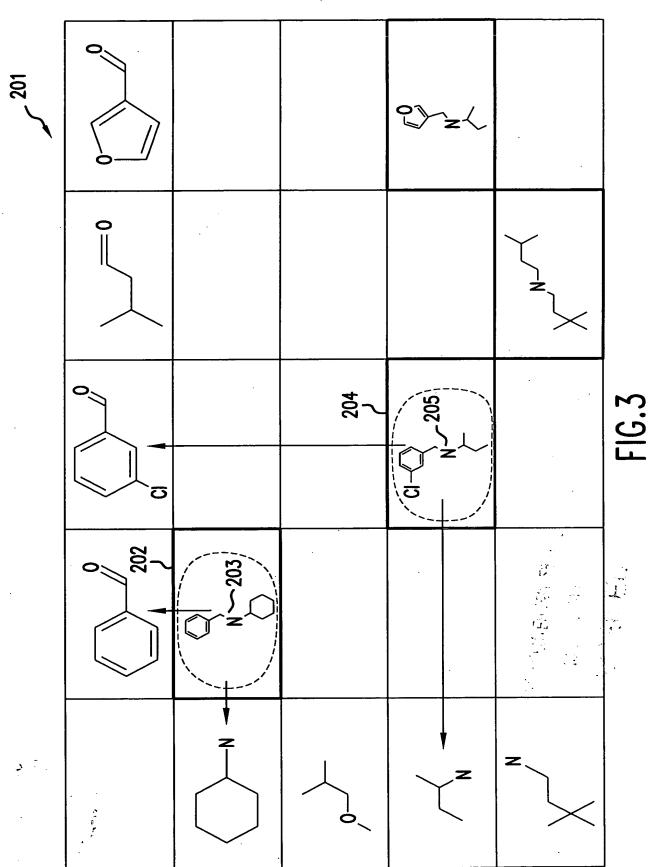
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DRAFTSMAN		

Appl. No. 09/506,741; Group Art Unit: 1631
Dkt. No. 1503.0730000;
Inventor(s): Lobanov et al.; Tel: 202/371-2600
Title: System, Method and Computer Program Product for Fast and Efficient Searching of Large Chemical Libraries

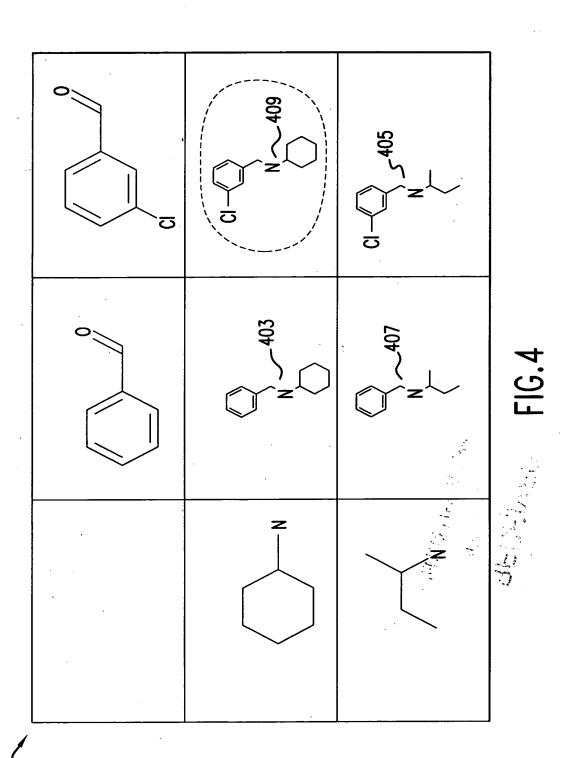
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APPROVED O.G. FIG. ΒY DRAFTSMAN

Appl. No. 09/506,741; Group Art Unit: 1631
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Title: System, Method and Computer Program Product for Fast and Efficient Searching of Large Chemical Libraries



Appl. No. 09/506,741; Group Art Unit: 1631
Dkt. No. 1503.0730000;
Inventor(s): Lobanov et al.; Tel: 202/371-2600
Title: System, Method and Computer Program Product for Fast and Efficient Searching of Large Chemical Libraries



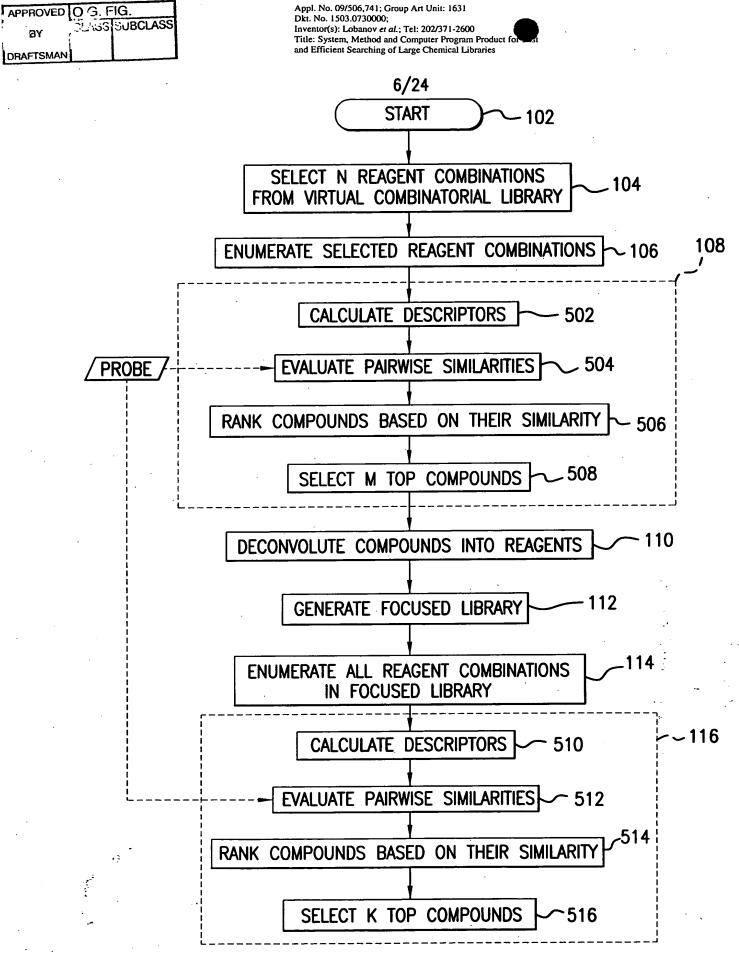


FIG.5

Sheet 7 of 24 APPROVED O G. FIG. Appl. No. 09/506,741; Group Art Unit: 1631 Dkt. No. 1503.0730000; CLISS SUBCLASS Inventor(s): Lobanov et al.; Tel: 202/371-2600
Title: System, Method and Computer Program Product for Fast and Efficient Searching of Large Chemical Libraries DRAFTSMAN 7/24 **START** - 102 SELECT N REAGENT COMBINATIONS 104 FROM VIRTUAL COMBINATORIAL LIBRARY 108 ENUMERATE SELECTED REAGENT COMBINATIONS CALCULATE DESCRIPTORS - 502 EVALUATE PAIRWISE SIMILARITIES **PROBE** RANK COMPOUNDS BASED ON THEIR SIMILARITY SELECT M TOP COMPOUNDS DECONVOLUTE COMPOUNDS INTO REAGENTS 12 GENERATE FOCUSED LIBRARY ENUMERATE ALL REAGENT COMBINATIONS

FIG.6

IN FOCUSED LIBRARY

CALCULATE DESCRIPTORS

SELECT SUB-MATRIX OF K COMPOUNDS

THAT INCLUDES ONLY T TOTAL REAGENTS

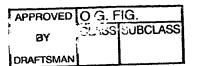
EVALUATE SIMILARITY OF SUB-MATRIX

REFINE SET OF K COMPOUNDS

**~116** 

612

614



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Dkt. No. 1503.0730000;
Inventor(s): Lobanov et al.; Tel: 202/371-2600
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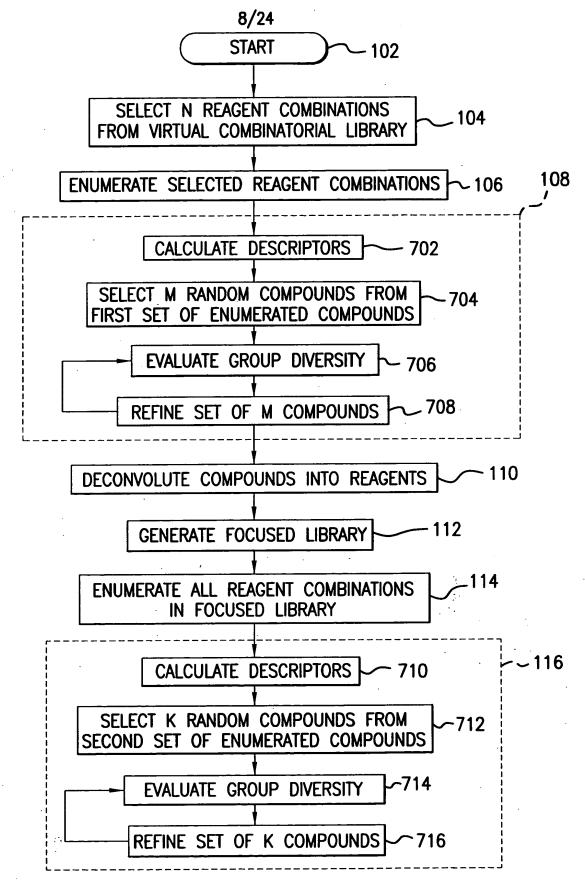


FIG.7

Appl. No. 09/506,741; Group Art Unit: 1631
Dkt. No. 1503.0730000;
Inventor(s): Lobanov et al.; Tel: 202/371-2600
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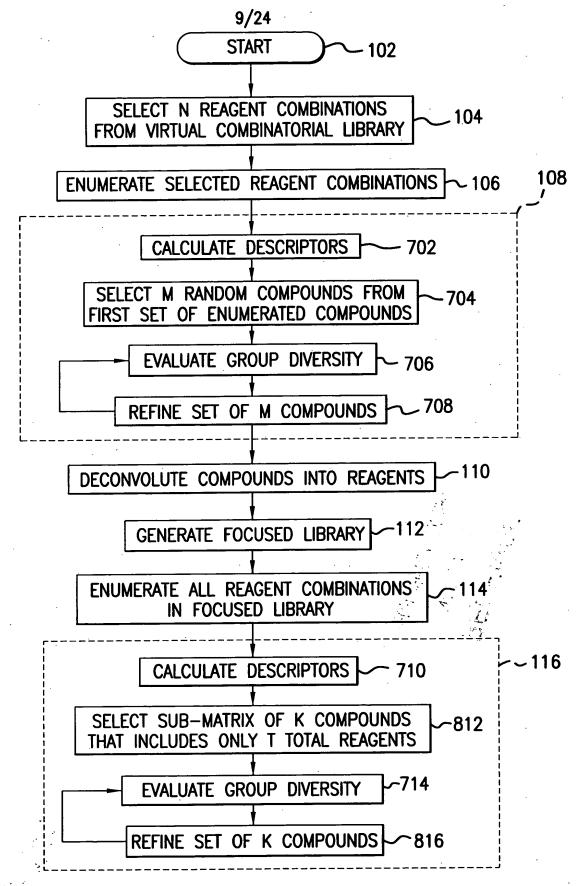


FIG.8

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Title: System, Method and Computer Program Product for Fast and Efficient Searching of Large Chemical Libraries

FIG.9A

FIG.9B

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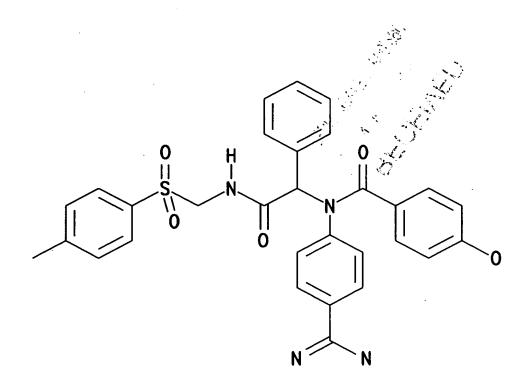
Appl. No. 09/506,741; Group Art Unit: 1631 Dkt. No. 1503.0730000; Inventor(s): Lobanov et al.; Tel: 202/371-2600 Title: System, Method and Computer Program Product for Fast and Efficient Searching of Large Chemical Libraries

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## ANTIARRHYTHMIC AGENT

FIG.10A



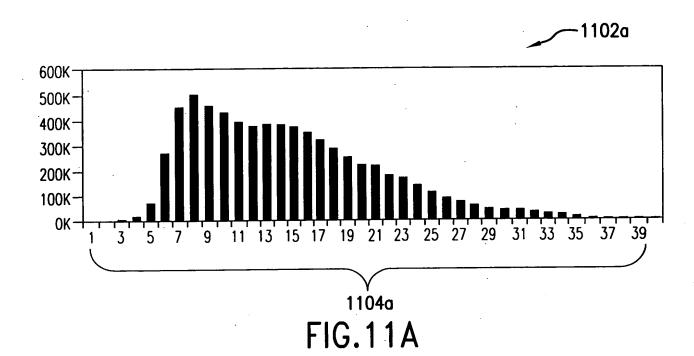
1.4 M THROMBIN INHIBITOR

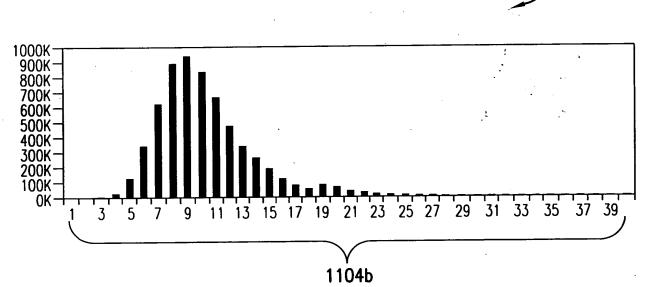
FIG.10B

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1102b

FIG.11B

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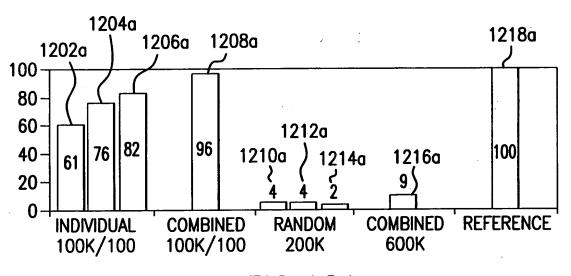


FIG.12A

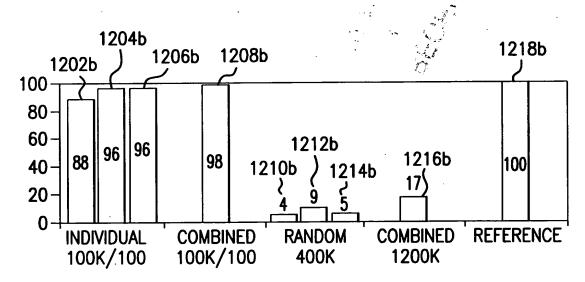


FIG.12B

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16.13

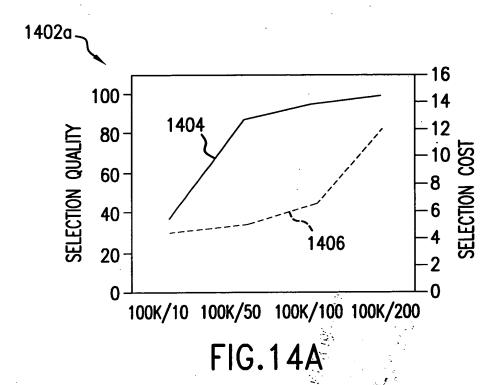
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į	PERCENT OF THE LIBRARY SCREENED	2	4	-2	_	15	12	9		2	6	2	2	တ	∞	45	62	78	∞	20	9	2	5	=======================================	2
	TOTAL COMPOUNDS SCREENED	6750000	300900	338688	442461	812877	832869	408747	442461	960669	000009	6290000	303459	588702	1101753	2831136	3904665	1780446	1101753	1268019	997959	601983	588702	804267	120000
	PERCENT OF TOP 100 FOUND	2	37	88	8	2	<b>æ</b>	8	96	98	6	2	46	8	88	88	2	97	88	5	88	32	9	88	-
	AVERAGE SIMILARITY	1.30034	1.48825	1.31148	1.30306	1.30034	1.32782	1,30141	1.30306	1.30306	1.82826	1.47494	1.78473	1.47494	1.47737	1.47737	1.47494	1.48308	1.47737	1.47494	1.52529	1.49912	1.47494	1.48086	7 18751
	SCORE SCORE	0.7662	0.8585	0.7662	0.7662	0.7662	0.7662	0.7662	0.7662	0.7662	1.1272	0.0000	0.7745	0.000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	UUUU U
	number of most Similar Compounds Selected	991	9	8	901	100	8	8	8	9	100	901	2	<b>5</b>	100	100	8	8	9	8	. 81	92	8	8	100
	SIZE OF FOCUSED	N/A	30.	12896	47487	170959	276623	126249	47487	33032	A/N	N/A	1153	96234	152/97	843712	1300555	583482	267251	222673	331653	190661	96234	68089	N/A
	number of Reagents	88	8	2	108	191	<u>동</u>	₹ <u></u>	<u>\$</u>	96	N/A	3)	23	76	66	139	151	121	66	96	102	88	9/	88	V/N
	Best Similarity Score	0.7662	1.0207	1.2266	1.0207	0.7662	2.1172	1.6919	1.0207	1.4557	1.1272	0.0000	0.7745	1.6871	1.4382	1.1581	2.5500	1.3793	1.4382	0.77448	2.50076	1.22499	1.6871	1.1667	00000
	NONNDS SEFECTED POUNDS SELECTED	100	2	20	100	200	2	8	5	100	100	901	<b>0</b>	S	100	200	2	5	901	9	22	S	22	50	130
	ZEFECLION ZIZE OŁ KYNDOW	N/A	10000	100000	100000	100000	<u>\$</u>	<u>\$</u>	10000	200000	200000	N/A	10000	10000	100000	100000	99	10000	100000	200000	1000	10000	100000	200000	400000
		DIAMINE LIBRARY	100K/10	00K/50	00K/100	100K/200	K/100	0K/100	100K/100	.00K/100	ANDOM 200K	lgi LIBRARY	00K/10	00K/50	00K/100	00K/200	K/100	0K/100	100K/100	00K/100	1K/50	OK/20	00K/50	00K/50	RANDOM 400K
ι		ب	_	_		_	_	_	_	7	اک ا	<u> </u>	=		7	<u> </u>	=	=	=	~	_	_		7	<u> </u>

Sheet 15 of 24

APPROVED O.G. FIG.
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DRAFTSMAN

Appl. No. 09/506,741; Group Art Unit: 1631 Dkt. No. 1503.0730000; Inventor(s): Lobanov et al.; Tel: 202/371-2600 Title: System, Method and Computer Program Product for Fast and Efficient Searching of Large Chemical Libraries



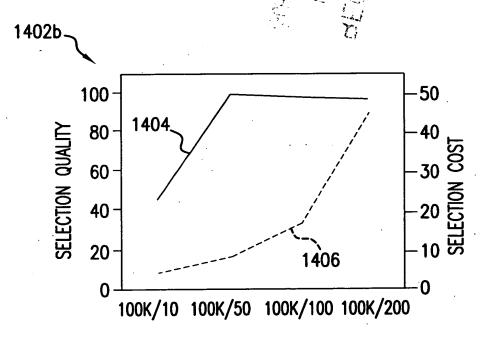
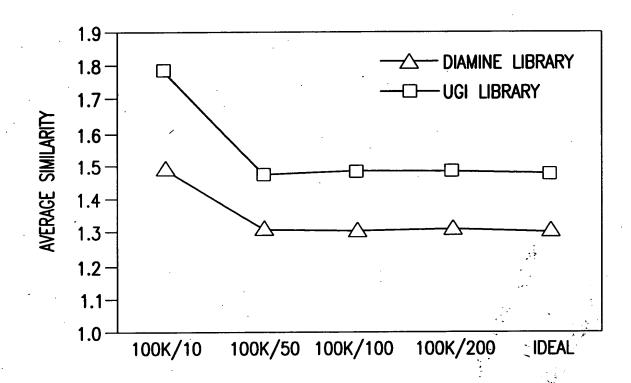


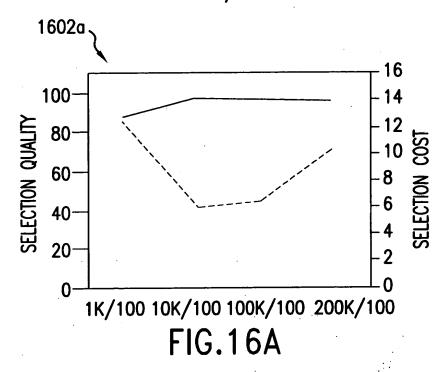
FIG.14B

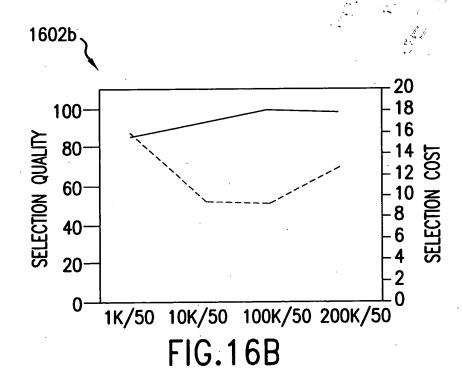
Appl. No. 09/506,741; Group Art Unit: 1631 Dkt. No. 1503.0730000; Inventor(s): Lobanov et al.; Tel: 202/371-2600 Title: System, Method and Computer Program Product for Fast and Efficient Searching of Large Chemical Libraries



**FIG.15** 

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Inventor(s): Lobanov et al.; Tel: 202/371-2600
Title: System, Method and Computer Program Product for Fast and Efficient Searching of Large Chemical Libraries

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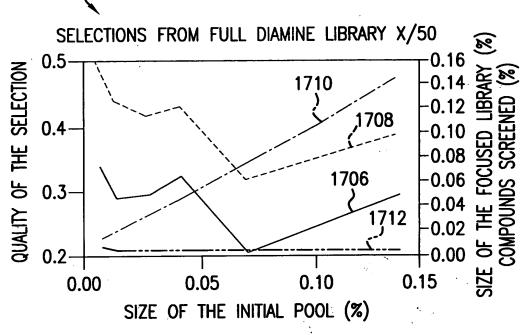
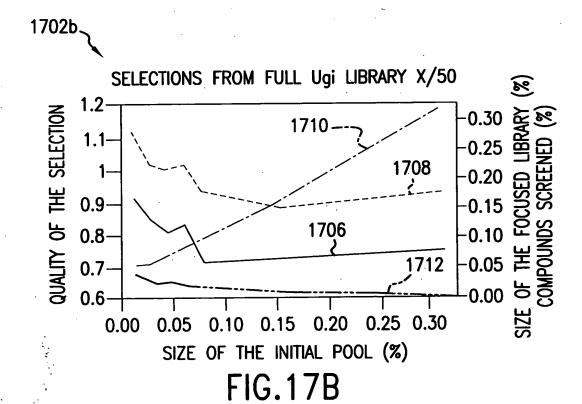
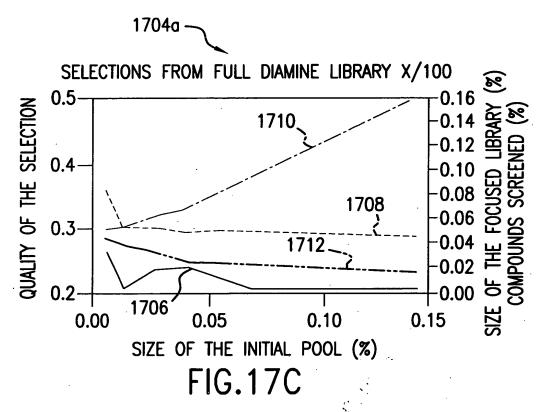
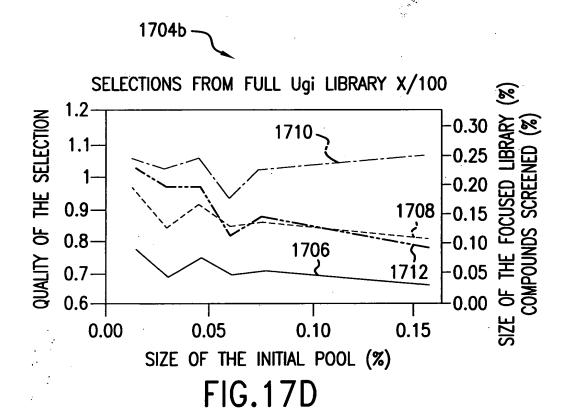


FIG.17A



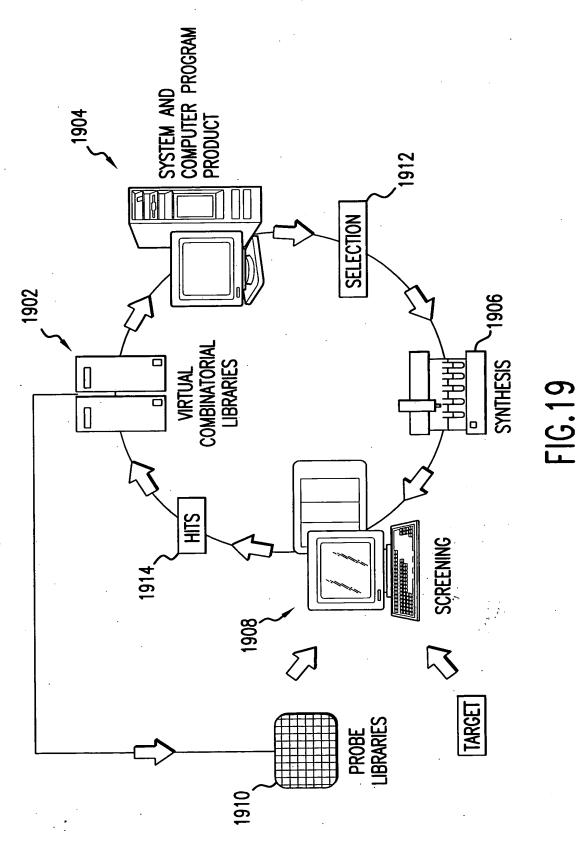
Appl. No. 09/506,741; Group Art Unit: 1631 Dkt. No. 1503.0730000; Inventor(s): Lobanov et al.; Tel: 202/371-2600 Title: System, Method and Computer Program Product for Fast and Efficient Searching of Large Chemical Libraries

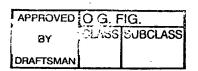




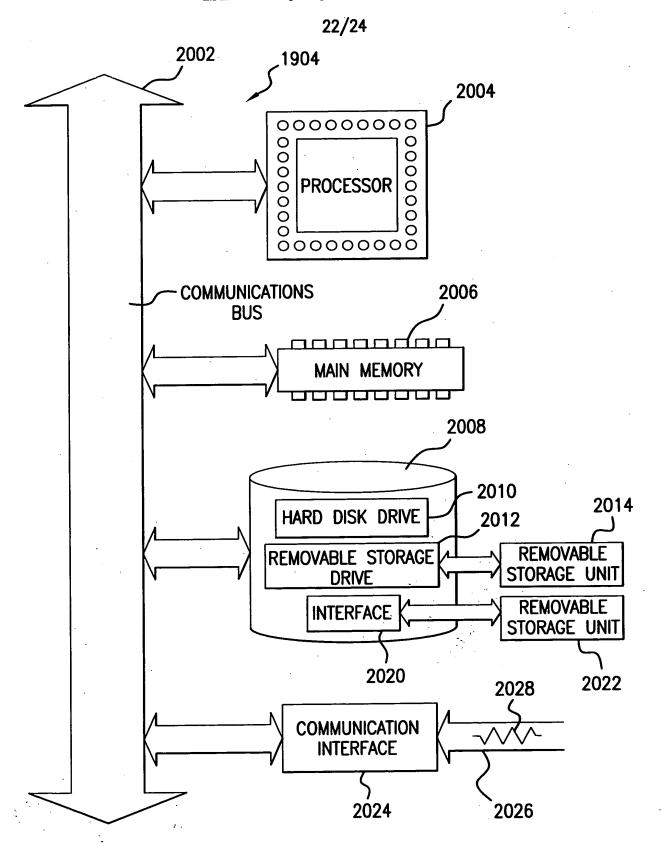
Appl. No. 09/506,741; Group Art Unit: 1631
Dkt. No. 1503.0730000;
Inventor(s): Lobanov et al.; Tel: 202/371-2600
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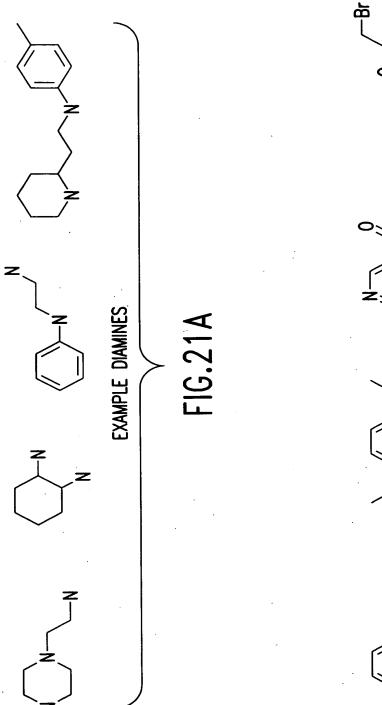
Appl. No. 09/506,741; Group Art Unit: 1631
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Inventor(s): Lobanov et al.; Tel: 202/371-2600
Title: System, Method and Computer Program Product for Fast and Efficient Searching of Large Chemical Libraries



**FIG.20** 

APPROVED O.G. FIG. DRAFTSMAN

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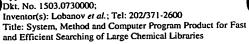




FIG.22A

FIG.22B

FIG.22C

FIG.22D